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SIMULATION OF ESPRESSO COFFEE EXTRACTION USING SMOOTHED PARTICLE HYDRODYNAMICS

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Abstract. A mesoscopic model for the simulation of espresso extraction based on the Smoothed Particle Hydrodynamics method is presented. The model incorporates some essential features such as bimodal granulometry (fines-coarses) of the coffee bed, double (liquid/intra-granular) molecular diffusion and solid-liquid release mechanism. The porous structures ('coarses') are modelled as stationary solid regions whereas the migration of cellular fragments ('fines') is described by single-particles advected by the flow. The boundary filter is modelled as a buffer region where fines are immobilized while entering it, therefore providing a transient flow impedance. The model captures well the transient permeability of the coffee bed under direct-inverse discharge observed in experiments, showing the importance of fines migration on the hydrodynamics of the extraction. The concentration kinetics for different molecular compounds are also studied. The present work lays down the basis for the virtual analysis of coffee flavors by monitoring the hydrodynamic and microstructural effects on the balance of extracted key-odorant or taste-actives compounds in the beverage.

1 INTRODUCTION

Coffee is one of the most widely consumed beverages in the world. Several brewing methods can be used to prepare the beverage depending on consumer's taste as well as cultural and geographical habits. In many countries, drip brew, or filter coffee, is the traditionally consumed beverage. This method for brewing coffee involves pouring water over roasted and ground coffee contained on a filter. Water seeps through the coffee, absorbing its extractable fraction solely under gravity, and then passes through the bottom of the filter. The used coffee grounds are retained in the filter with the liquid falling (dripping) into a collecting vessel such as a carafe or pot. In addition to this popular coffee beverage, espresso coffee is gaining a big world-wide success not only as a phenomenon of

fashion. This is also due to the greater sensory satisfaction it gives to the consumer when compared with coffees prepared with other brewing methods [1]. Traditional espresso brewing requires specialized equipments that have to heat water to a temperature between 92C and 94C and pressurize it to 9 ± 2 bar. The process is applied (percolation time) until the beverage volume in the cup meets consumer's personal preference or the regional traditions. For example, in Italy, the volume ranges from 20 mL or less (ristretto) to 50 mL or more (lungo), with a typical volume of 20 to 30 mL for regular espresso shot [2]. The application of pressure, makes espresso brewing more complex than drip brewing from a physico-chemical process point of view [3]. In particular, during the passage of hot water through the layer of roasted and ground coffee (coffee bed), the following chemical and physical phenomena can be described [4]: (A) *Initial imbibition* of the porous coffee matrix with consequent irreversible progressive swelling of the coffee particles, this causes a progressive decrease in the porosity of the matrix and therefore an increase in hydraulic resistance. During this process, reversible migration of small coffee particles in the direction of water flow also occurs. (B) *Solubilization* of the hydrophilic substances contained in the coffee bed resulting in a progressive increase of density and viscosity of the percolating fluid flow and the concomitant partial erosion of the coffee particles. (C) *Stripping* of coffee lipids thanks to the pressurized hot water and progressive emulsification of lipophilic substances due to the action of surfactants naturally occurring in roasted coffee, with a further progressive increase in viscosity of the percolating fluid.
From a coffee cup quality point of view, in addition to model the physics of the espresso extraction, it is necessary to take into the account the modelling of the mass transfer during the process and preferably, the taste-wise chemical compounds mass transfer in order to follow the extraction of solubles (and if possible also of not-solubles) from roasted coffee.

The goal of this work is to provide a novel simulation framework based on the Smoothed Particle Hydrodynamic (SPH) method to describe coffee espresso extraction taking into account the complex mesoscopic structure of the coffee bed. SPH is a popular Lagrangian method to resolve the flow of simple and complex liquids by relying on an kernel-based discretization of prescribed set of partial differential equations (e.g. Navier-Stokes equations for the momentum, advection-diffusion equation for suspended solute etc.) describing the flow locally. This generally leads to a discrete set of ordinary differential equations for fluid particles interacting pair-wisely [5]. Due to its Lagrangian meshless character the technique is able to tackle complex geometries, such as those arising in a deformable porous media, as well as to model Lagrangian particulate transport [6], memory effects in complex fluids [7] and multiphase flow [8] in a natural way . The technique has been also generalized to incorporate Brownian fluctuations (when needed) on hydrodynamic variables by using the so-called GENERIC framework (an acronym for General Equation for Non-equilibrium Reversible-Irreversible Coupling) [9]. This has allowed it to be extended to the regime of fluctuating hydrodynamics both for simple [10] and complex non-Newtonian fluids [11].
In this work we present a new SPH model of coffee filtration able to describe the entire complex mesoscopic structure of the coffee bed and its potential influence on the flow of the

liquid through the filter as well as the transport/release of solute. Complex granulometry of the coffee bed is described on different scales, from the fixed porous medium represented by the large solid grains, to the small free cellular fragments - i.e. the 'fines' - down to the molecular solute (e.g. caffeine) modelled via a concentration field. Moreover, for the dynamics of the molecular solute within liquid phase is taken into account together with a mass transfer model due to stripping from the solid-liquid interface. The mesoscopic model naturally leads to the transient flow permeability effects observed in experiments [12] - as well as its effect on the concentration dynamics - which have been traditionally interpreted in terms of microstructural changes such as pore's swelling or fines particles migration [13]. An extended model fully coupled with intra-granular transport of solute has been recently presented in [14].

2 MESOSCOPIC PARTICLE MODEL

In this section the mesoscopic model of coffee filtration is presented. The solid phases will be modelled based on the different characteristic dimensions of the specific components. In particular, in the problem of coffee filtration three main characteristic dimensions are associated to distinct dispersed phases: (i) solid grains (≈450 μm) representing the fixed porous structure; (ii) the so-called 'fines' (≈30 μm) representing the flowing cellular fragments and (iii) the molecular components, e.g. volatile or non volatile compounds such as caffeine etc. (≈ 1-10 nm). Water flowing through the porous structure and coupled with material transport will be modelled based on standard Newtonian hydrodynamics. A sketch of the model is given in Fig. (1).

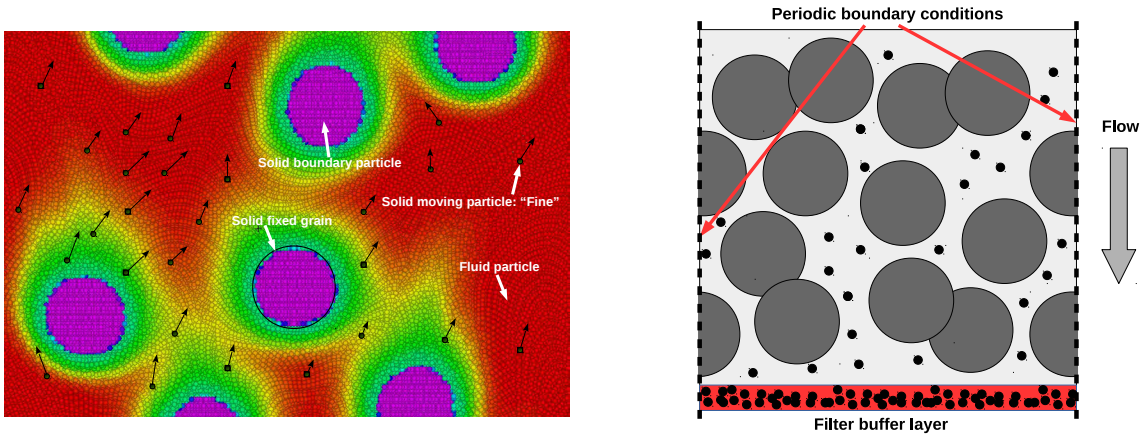

Figure 1: Left: sketch of the SPH model. Solid dispersed phases is described at different levels. (a) Large solid grains representing the fixed porous structures are denoted as violet regions. (b) Small solid fragments, i.e. the "fines", are modelled as independent solid moving particles. (c) The smallest dispersed molecular components - the chemical species - are treated on a continuum level via a concentration field (color map). Right: sketch of the filter model. Fines are advected by the flow. Filter is modelled as a buffer region (red area in the figure) of specified thickness. When fines enter this region they are 'immobilized' and provide transient mechanical impedance depending on the instantaneous concentration of trapped fines.

2.1 Suspending fluid phase model: Smoothed Particle Hydrodynamics

The fluid phase dynamics is governed by the isothermal Navier-Stokes equations. The model adopted in this work is the Smoothed Particle Hydrodynamics (SPH) which is a Lagrangian meshless method for the numerical solution of partial differential equations [5]. In SPH a set of fluid particles $i = 1, .., N$ are distributed homogeneously over the domain and move according to conservative and dissipative interparticle forces $\mathbf{F}_{ij}^{C,D}$ estimated from their local neighborhood. In the isothermal case, the following set of ordinary differential equations for the particle positions, velocities are solved numerically and represent a Lagrangian discretization of the Navier-Stokes equations [5]

$$\dot{\mathbf{r}}_i = \mathbf{v}_i, \qquad m\dot{\mathbf{v}}_i = \underbrace{-\sum_j \overbrace{\left(\frac{p_i}{d_i^2} + \frac{p_j}{d_j^2}\right) W'_{ij}\mathbf{e}_{ij}}^{\mathbf{F}_{ij}^C}}_{(\nabla p/\rho)_i} + \underbrace{4\sum_j \overbrace{\bar{\eta}_{ij}\frac{W'_{ij}}{d_i d_j r_{ij}}\mathbf{v}_{ij}}^{\mathbf{F}_{ij}^D}}_{\eta(\nabla^2\mathbf{v}/\rho)_i} + \mathbf{g}_i, \qquad (1)$$

where the time derivative is Lagrangian and $W_{ij} = W(r = r_{ij})$ is a kernel function and $W'_{ij} = \partial W(r)/\partial r|_{r=r_{ij}}$ its spatial derivative. $r_{ij} = \|\mathbf{r}_{ij}\| = \|\mathbf{r}_i - \mathbf{r}_j\|$, $\mathbf{e}_{ij} = \mathbf{r}_{ij}/r_{ij}$ is the unit vector joining particles i and j, whereas $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ their corresponding velocity difference. $\bar{\eta}_{ij} = (\eta_i + \eta_j)/2$ is the averaged dynamic viscosity of the fluid and η_i is the local value of viscosity associated to particle i. p_i represents the pressure associated to particle i, calculated via a suitable equation of state (EOS). Here we choose an ideal EOS $p_i = c_s^2(\rho_i - \rho_0)$ where $\rho_i = md_i$ is the mass density associated to the particle i (m is the constant particle mass) and c_s is the sound speed in the liquid. $d_i = \sum_j W_{ij}$ is the corresponding number density and $\mathbf{g}_i$ represents any external body force. Finally, in the previous expression for the EOS the speed of sounds c_s must be chosen sufficiently larger than any other velocity present in the problem in order to avoid artificial compressibility effects [5]. The SPH model can be generalized to fluctuating hydrodynamics by casting it into the so-called GENERIC formulation [9] which allows to incorporate additional stochastic terms in Eq.(1) satisfying Fluctuation-Dissipation Theorem [10].

2.2 Porous solid phase model

Solid regions of arbitrary shapes can be created by immobilizing a certain number of solid SPH particles located within a prescribed fixed porous structure (i.e. the solid coffee grains) in a similar way to what done in [15] (see Fig.1 left). No-slip velocity condition is enforced on the liquid-solid interface where boundary particle velocities are set to zero. Solid SPH particles (violet in the figure) interact with fluid SPH particles by means of the same forces presented in Eq.(1), but differently to fluid particles, they are not allowed to move.

2.3 Dispersed molecular phase continuum model

Due to the large scale separation existing between molecular compounds (e.g. caffeine: $\approx$ 1nm) and the solid grains forming the porous structure ($\approx 450\mu$m), the dispersed

molecular phase can be treated as a continuum and modelled through a concentration field. In this case, each SPH fluid particle is equipped with an additional microstructural variable, i.e. a scalar concentration field c_i, whose dynamics is governed by an inhomogeneous advection-diffusion equation. We consider here the most general case where the diffusion coefficient $D(\mathbf{r})$ can be space-dependent. The corresponding Lagrangian SPH discretization reads

$$\dot{c}_i = \underbrace{4\sum_j \bar{D}_{i,j}\frac{W'_{ij}}{d_i d_j}\frac{c_{ij}}{r_{ij}}}_{D(\nabla^2 c)_i} \tag{2}$$

where the time derivative is Lagrangian and $c_{ij} = c_i - c_j$ and $\bar{D}_{i,j} = (D_i + D_j)/2$ is the average interparticle diffusion coefficient and D_i is the local diffusion coefficient associated to particle i. Note that advection is implicitly taken into account through the Lagrangian motion of the particles. Note also that the term within the summation in Eq.(2) is anti-symmetric by swapping i, j indices and therefore the mass of solute is automatically conserved. Fig. (1) shows a color map describing a frame of the concentration field of a given molecular compound released from the solid grains (violet: maximum - red: zero). Note that different $\bar{D}_{i,j}$ values can be associated to different SPH particles-pairs: this is important, for example, to model the diffusive molecular processes, separately, in the liquid phase and within the solid grain. In practice, several volatile or non-volatile taste-active compounds with different diffusional properties are associated to the final sensorial experience (fruity, malty, honey-like, buttery, roasty etc.). In the process of coffee filtration it is therefore important to assess the instantaneous time-dependent concentration of different compounds (i.e. characterized by different $D_{b,s}$) in the cup, in order to optimize the product and/or target specific flavors [16].

2.4 Discrete "fines" model

"Fines" are modelled as single solid SPH particles advected by the flow. We adopt here the so-called *minimal single-particle model* proposed in the context of Dissipative Particle Dynamics [17]. We select randomly a number of SPH particles in the fluid domain and, according to the target fines concentration, we regard them as a solid flowing particles (black spheres in Fig. (1)). It should be noted that in the bulk flow the fines are just passive tracers and do not have any influence on the flow. However, if their positions are constrained they are characterized by a well-defined hydrodynamic radius (approximately equal to the kernel cutoff radius r_c) and therefore they provide a mechanism of mechanical impedance for the bulk flow itself. This feature is important in the model of the physical filter.

2.5 Filter model

The filter at the bottom (or upper) boundary of the coffee bed is modelled as an additional buffer region of finite thickness (red area in Fig. 1: right). The fines move with the flow under the action of an external pressure force and eventually percolate the porous structure; when they finally enter the bottom buffer region, their identity change

and they are regarded as fixed solid boundary particles with zero velocity - of the same type of those used to model the solid region inside a grain (see Fig. 1 left). As a consequence, they present an obstacle to the flow of the down-streaming fluid particles which exit the domain. Depending on the initial concentration of fines dispersed in the liquid domain (denoted as θ) the total number of fines trapped in the filter can significantly change together with the values of filter resistance leading to a simple model of transient coffee bed permeability [12].

3 NUMERICAL RESULTS

3.1 Numerical parameters

In order to model numerically the physical system discussed above, we chose the following setup. (A) **Coarse coffee grains** ('coarses': 500μm) : they are modelled as fixed spherical solid regions of size $d_{grain} = 2.0$ using 16 SPH particles per diameter (see Fig. 1). The 'coarses' solid volume fraction is $\phi = 0.48$. (B) **Fine particles** ('fines': 30μm): they are modelled as mobile single SPH particles (passive tracers). Being the SPH resolution of the grain 16, we have a computational ratio $d_{grain}/d_{fine} \approx 16$ ($d_{fine} \approx$ hydrodynamic radius SPH particle) which is consistent with the physical ration in real coffee bed. The 'fines' solid volume fraction will range in $\theta = 0.001 - 0.01$. (C) **Molecular compounds** (e.g. caffeine, hyperfines etc.: $\ll 1\mu$m). Their small size compared to the other characteristic lengths (H, d_{grain}, d_{fine}) justifies a continuum approach based on the solution of an advection-diffusion equation for the corresponding concentration field (Eq.(2)). Different species can in principle have different size and therefore different bulk diffusion coefficients D_b as well as release rates D_r. (D) **Coffee bed** (2cm thickness):to model a realistic coffee bed of, say, 2cm thickness[18] we consider a height of the simulation domain $L_y = 80$ (y is the direction of filtration), leading to a numerical ratio $L_y/d_{grain} = 40$. In the transversal direction (x) it is assumed that the coffee bed is homogeneous and periodic boundary conditions can be imposed. This allows to minimize the size of the simulation domain and computing time. Finite size effects can be eliminated by taking $L_x = 10 = 5d_{fine}$. In conclusion, we consider a two-dimensional domain $L_x \times L_y = 10 \times 80$, discretized with $N = 80 \times 640 = 51,200$ SPH particles.

Fluid density is chosen to be $\rho = 1$, whereas viscosity $\mu = 3$. The average flow velocity (which controls the effective Reynolds number) is tuned by applying an effective body acceleration mimicking a pressure drop, i.e. $F = \Delta p/(L_y\rho)$. For example, a value of $F = 2000$ leads to peak average velocity $V_{max} \approx 15$ and peak Reynolds number (in absence of fines: just fixed solid grains) $\mathrm{Re}_{max} = d_{grain}V_{max}\rho/\eta \approx 10$, matching experimental conditions. The speed of sound is chosen sufficiently large than V_{max} to reduce density fluctuations, i.e. $c_s = 500 \gg V_{max}$. Finally, the bulk diffusion coefficient for a specific compound will range in $D_b = 0.005 - 0.1$ to give a bulk Peclet number $\mathrm{Pe} = 600 - 6000$ corresponding to transient peak flow velocity. Values for the corresponding rate of of release coefficients will be typically a factor 10 smaller than the the bulk free diffusion, i.e. $D_r = 0.001 - 0.1$, but different conditions will be explored.

3.2 Inverse filtration process: transient permeability

In order to understand the different transport processes involved in the percolation of water through the coffee bed system, a transient direct/inverse filtration is considered and results are discussed in relation to experimental data [18]. In this section we focus on the hydrodynamic response of the system. In particular, Fig.2 shows the dynamics

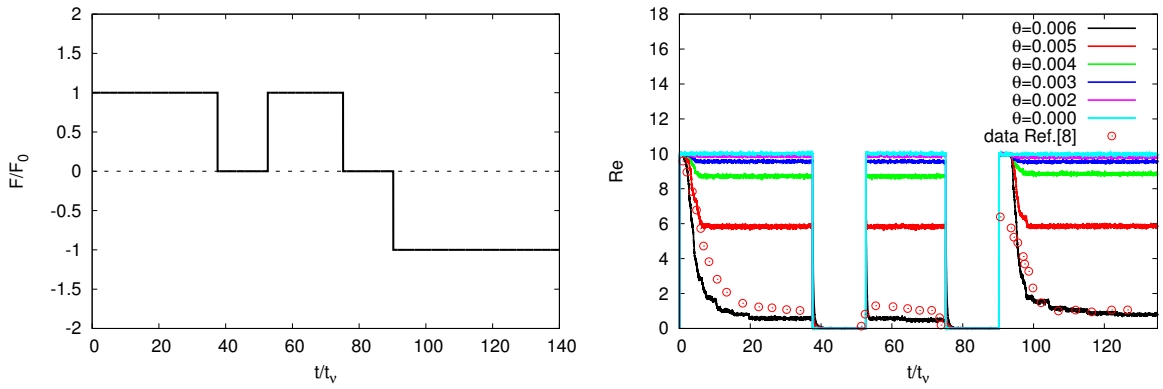

Figure 2: Inverse discharge. Left: time-dependent dimensionless applied forcing. Right: time-dependent Reynolds number (absolute value) for different fines concentration θ. Slow permeability decay is evident as result of increase fine concentration.

of the full direct/inverse discharge. Left: the time-dependent dimensionless forcing (i.e. pressure drop). Right: time-dependent Reynolds number based on spatially-averaged flow velocity (absolute value) for different fines-concentration θ. Experimental data for the transient direct/inverse discharge flow reported in [13] have been also showed as reference. Note that in the experimental data the initial transient flow increase have been removed since (in experiment) it is due to an applied pressure raising over a finite time, i.e. not 'instantaneously' applied as in the simulations. Time has been made dimensionless with the viscous liquid time $\tau_\nu = d^2_{grain}/\nu = 2^2/3 = 1.33$. In order to compare with experiments, corresponding real viscous time in SI units should be $\tau_\nu = d^2_{grain}/\nu = (400 \times 10^{-6})^2/10^{-6} = 0.16$s.

Initially a *direct discharge* process with constant pressure forcing is applied up to dimensionless times approximately equal to $t^* = t/\tau_\nu = 38$. This is followed by a resting state (zero applied force for t^*=38-55) after which the same constant forcing is applied again. Finally, an additional resting condition (t^*=75-90) is followed by a constant pressure force applied in the opposite direction (*inverse discharge*).

We consider first the flow response of the pure porous structure, i.e. for fine concentration $\theta = 0$ (light blue line in Fig.2). After application of pressure drop, flow rate increases quickly and reaches a steady state value (Re $\approx$ 10). The small transient at $\theta = 0$ (not visible in the figure) occurs on typical viscous time scales of order τ_ν. After removal of the forcing, flow rates decay quickly to zero (relaxation time scales $\approx \tau_\nu$) and then again reach the same value upon re-activation of the forcing in the same direction. After forcing reversal, again the flow responds very quickly reaching the same value of the Reynolds

number (absolute value is shown in the figure). Under these conditions ($\theta = 0$), coffee bed permeability is constant and the results are in agreement with previous simulations. The case where fines are present ($\theta \neq 0$) is, however, qualitatively different. We have studied different fine concentrations ranging from 0.002 to 0.006 as shown in Fig.2 (right). Initially (direct discharge at $t^* < 3$) the flow reaches the same peak Reynolds number during the very short viscous time scales. This again corresponds to the fast viscous relaxation consistent with a fixed porous structure. In this case, however, it does not represent a steady state but a transient peak. In fact, the meta-stable state at Re=10 is followed by a transient decay characterized by a significant longer relaxation time compared to τ_ν. This slow decay ($3 < t^* < 10$) is due to the fines be displaced and their transient accumulation in the filter. In fact, fines need some finite time to migrate from their initial positions (randomly dispersed in the liquid phase) to the filter at the boundary of the domain. As the number of trapped particles increases, so does the overall flow resistance leading to the observed transient permeability.
Flow rate eventually reaches a steady-state value which depends on the initial concentration of fines present in the liquid phase. Small values of $\theta = 0.001$ (violet line) do not alter significant the filtration hydrodynamics respect to simple fixed porous case. However, $\theta = 0.006$ (black line) leads to a significant reduction of flow permeability (nearly one order in the averaged steady Reynolds number) in substantial agreement with experimental data of espresso extraction reported in Ref.[18].
If the forcing term is temporarily switched off and then re-activated, the flow rate reaches instantaneously the same steady state. This means that the water flows through the same geometrical configuration corresponding to the fixed porous structure with an additional mechanical impedance offered by the unchanged amount of fines trapped in the filter. Finally, if we invert the flow we observe again the same relaxation process characterized by the long relaxation time as at the beginning of the simulation. The reversed flow forces the fines to move in the opposite direction and be released by the filter, i.e. again through the coffee bed. A typical dimensionless time $\tau_m^* \approx H/(V_{max}\tau_\nu) = 7.1$ is required for all fines to migrate towards the bottom filter, after which the permeability reaches again a steady state. This is in remarkable good agreement with the transient decay observed in Fig.2 (right) and in experiment of inverse coffee discharge. These results show that fines migration is the main mesoscopic transport process responsible for the reversible transient permeability observed in experiments [13, 12, 18].

3.3 Concentration dynamics

After validation of the hydrodynamic response and transient permeability made in the previous section, we study here the release and dynamics of a passive scalar field (the molecular compound concentration, e.g. caffeine) during the filtration process. In particular, we are interested in the resulting *cumulative output concentration* in the cup for different choice of physical parameters, namely the concentration of fines θ, the bulk diffusion coefficients D_b of the molecular compound and release rates D_r. In this work intra-granular diffusion coefficients D_s is set to zero.

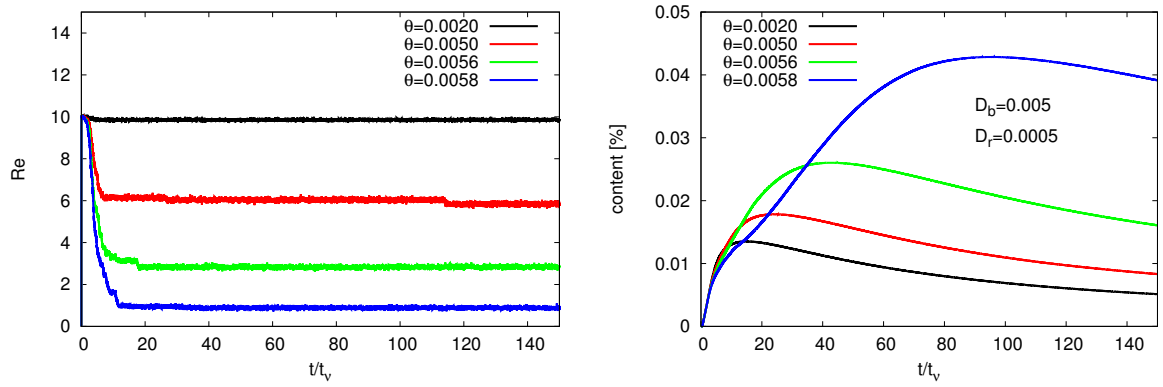

Figure 3: Direct discharge. Left: time-dependent Reynolds number (absolute value) for different fines concentration θ. Right: cumulative output concentration.

The cumulative output concentration is defined as compound-to-total mass ratio, i.e. $M_{compound}(t)/M_{tot}(t)$, where both quantities refer to the instantaneous values collected at the output and depend on time. We consider here the case of direct discharge (Fig.3: left). According to the time scale shown Fig.3, the temporal window explored is in the range of [0-25]s when dimensionalized by $\tau_\nu = 0.16s$, which corresponds to the typical time for an espresso preparation.

3.3.1 Effect of fine concentration θ

We first select two typical values of diffusion coefficients consistent with the discussion given in Sec.III.A, that is $D_b = 0.005$ (corresponding to peak/steady Peclet numbers Pe_{bulk} =6000/600) and $D_r = 0.0005 = 0.1D_b$, and check the effect of the fines concentration θ on the the cumulative molecular concentration. In this work intra-granular diffusion coefficients $D_s = 0$ so release mechanism is limited to the molecular compounds located inside a grain near the solid/liquid interface. Effect of different intra-granular diffusion coefficients D_s have been discussed in [14].
From Fig.3 (left) it can be seen how for small values of the fines concentration (e.g. $\theta = 0.002$) no transient permeability is observed. The resulting dynamics of the output compound concentration (Fig.3: right) exhibits a peak value ($\approx 1.4\%$) at short times ($t^* \approx 15$) after which the output compound concentration in the cup decreases softly. This peak value is shifted towards larger times and increases in magnitude for increasing θ. For example, for $\theta = 0.0058$, peak concentration ($\approx 4\%$) is reached at dimensionless time $t^* \approx 95$. Therefore, the present results shows that incorporation of a finite amount of fines, by inducing a transient permeability of the coffee bed, leads to smaller steady flow rates during filtration (Re ≈ 1). This, in turn, increases the residence time of the flow in contact with the solid surface of grains, therefore maximizing the molecular release process. In the case of fast flow (Re ≈ 10 for $\theta = 0.002$), water is washed quickly through the coffee bed preventing a proper release of substances into the fluid.

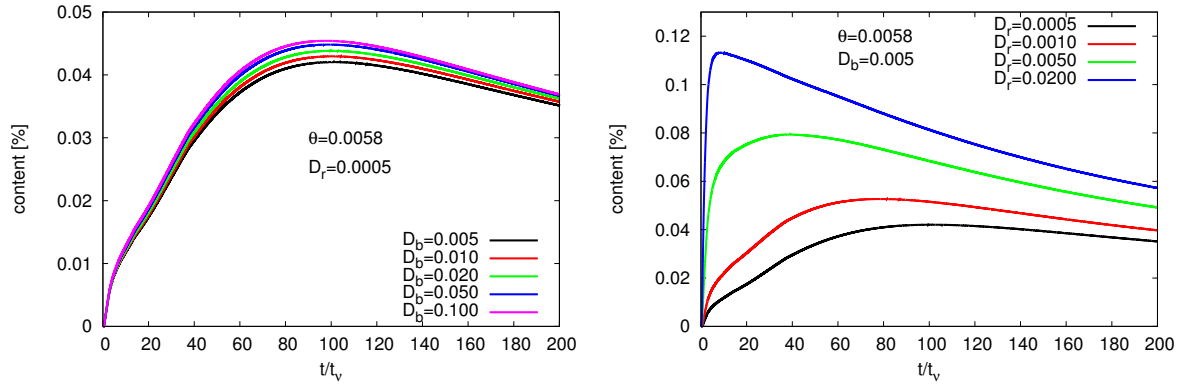

Figure 4: Direct discharge. Left: cumulative output caffeine concentration for fixed solid grain's release rate $D_r = 0.0005$ and $\theta = 0.0058$. Right: cumulative output caffeine concentration for fixed bulk diffusion $D_r = 0.0005$ and $\theta = 0.0058$.

3.3.2 Effect of bulk diffusion coefficient D_b and release rate D_r

In a second stage, we focus on the system with fines concentration $\theta = 0.0058$ (blue line in Fig.3) which reproduces reasonably well the transient flow rate reported in experiments with coffee filtration [13], i.e. a peak/minimal Reynolds numbers $\mathrm{Re} \approx 10 - 1$.
In Fig.4 we look at the effect of several parameters on the resulting output cumulative molecular concentration. In particular, in Fig.4 (left) the cumulative output concentration is shown for fixed solid grain's release rate $D_r = 0.0005$ and different bulk diffusion coefficients $D_b \in [0.005 : 0.1]$, spanning nearly two orders of magnitude in the bulk molecular Peclet number. It can be seen that D_b has only a minor effect on the final output concentration. There is a small consistent increase (less than 5%) in the peak for increasing D_b which can be attributed to difference in the release of molecular compounds in areas of stagnating flow. For molecular species released in these areas, the only possible mechanism of escape is by molecular diffusion, i.e. by slowly diffusing into region of large flow where the material is efficiently advected.

More interesting is the effect of the solid/liquid molecular release rate D_r on the cumulative output concentration (Fig.4: right). Here we consider a molecular compound with fixed bulk diffusion $D_b = 0.005$ at fine concentration $\theta = 0.0058$ and look at different release rates coefficients $D_r \in [0.0005 : 0.02]$. It is clear that D_r is the most relevant parameter controlling the final concentration of substance in the cup. For small values of the release coefficient (e.g $D_r = 0.0005$: black line) only a small peak (4%) is reached at relatively long times after which the cumulative concentration decay very slowly. On the other hand, large values of D_r (e.g $D_r = 0.02$: blue line) lead to a peak in the order of 12%. Moreover, all the material is released very efficiently in the very early stage of filtration ($t^* < 30$) with significant decay occurring later on. Maximization of molecular concentration in the cup can be therefore reached on extremely fast filtration processes by tuning the release mechanism. This is independent on the molecular property of the substance in the fluid (i.e. the diffusion coefficient D_b in water). However, it depends

strongly on D_r and can also depend on the intra-granular diffusion coefficient D_s of the molecular compound which indirectly affects D_r.

It is interesting to note that different compounds (i.e. different release coefficients) are clearly characterized by distinct kinetics which suggests that, depending on molecular specificity, the balance between different compounds is altered if extraction is stopped at different times. Because different compounds are tightly connected to specific flavors, and being taste perception a highly non-linear process [19], only minor changes in this delicate balance can lead to very different sensorial experience. For example caffeine and trigonelline are typically associated to degree of bitterness, whereas chlorogenic acids to acidic taste. These results indicate clearly that different preparation time for espresso can potentially lead to significant changes in taste perception and therefore the current framework can pave the way for a better flavor-engineering of espresso [14].

4 CONCLUSIONS

We have presented a SPH model for the simulation of espresso extraction which incorporates some essential physical features, i.e. (i) bimodal granulometry; (ii) double porosity model of molecular concentrations dynamics (enabling liquid-bulk and intra-granular solid diffusion); (iii) stripping mechanism of solid/liquid molecular release; and (iv) a model of mechanical filter. The correct transient permeability of the coffee bed has been reproduced under direct-inverse discharge conditions, showing the importance of fines migration on the hydrodynamic properties of the percolation and extraction process. Concentration dynamics for different molecular compounds have been studied. It was shown that the presence of the fines, leading to larger flow resistance leads to a dramatic increase of the residence time of water near the grain surface, therefore maximizing the release process. The long-term goal of this work is to use the current framework to control coffee flavors by monitoring the balance of specific taste-actives compound in the beverage.

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